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FINAL REPORT

Office of Naval Research

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for

Partial Funding of Gordon Research Conference

"Fundamental Interactions of Water with Solid Surfaces"

July 16-20, 1990

Kimball Union Academy

Meriden, NH

SEP 21 1994

94-30234

Submitted by:

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#### 1990 Gordon Research Conference on

#### "Fundamental Interactions of Water with Solid Surfaces"

The Gordon Conference on the "Fundamental Interactions of Water with Solid Surfaces" was held from July 16 to 20, 1990 at the Kimball Union Academy in Meriden, NH. The Chairman was Theodore E. Madey of Rutgers University; the Vice-Chairperson was Patricia A. Thiel of Iowa State University. The conference attracted sixty participants; about twenty five percent were from foreign countries, including Canada. There was a good mixture of scientists from universities, national laboratories and private industries, including young scientists and graduate students as well as established scientists.

The program brought together people working in rather different areas, including surface chemistry and physics, electrochemistry, corrosion, wetting, fracture, and processing of semiconductors. The program included eighteen lecturers and nine discussion leaders. The discussion following the talks was unusually active and stimulating, and a large percentage of the attendees contributed to the discussion.

There were a number of exciting new results presented and discussed. P. Norton presented high sensitivity reflection infrared absorption spectroscopic measurements of H<sub>2</sub>O on Ni(110), and correlated his results with absolute coverage determinations. Bonzel and White discussed the role of surface additive atoms on the structure and chemistry of H<sub>2</sub>C; and demonstrated that a "critical coverage" of adsorbed alkali is necessary for H<sub>2</sub>O dissociation to occur. Molecular dynamics simulations of H<sub>2</sub>O on metal and oxide surfaces were well covered by Spohr and Garofalini, and their results provided new insights into the structure and reactivity of adsorbed H<sub>2</sub>O. Stuve and Wagner described the linkage between surface science and electrochemistry in H<sub>2</sub>O-solid interactions, and Wagner reported positive evidence for adsorbed hydronium, H<sub>3</sub>O. Chabal described the use of aqueous HF for producing atomically smooth and clean Si(111) surfaces, and Sinclair described the problems caused by moisture in failure of semiconductor electronics.

The role of moisture in fracture of brittle materials was discussed by Lawn, and Porter presented exciting evidence for the structure of  $\rm H_2O$  layers between two surfaces at distances of the order 1 nm. Dubois provided the first convincing data showing the relation between surface science (thermal desorption) measurements and macroscopic wetting of surfaces. Finally, Campbell and Kasemo described detailed kinetic schemes for the formation and decomposition of  $\rm H_2O$ .

DIC QUALITY DISCLARA

There were two poster sessions ining a total of twenty four posters of high calibre. All reports I rece\_\_eq indicated that the conference was successful and stimulating. The next Gordon Conference on this subject will be scheduled in four to five years, under the chairmanship of Prof. Patricia Thiel, Iowa State University.

#### Attachments:

- 1. Conference Program
- 2. List of Poster Presentations
- 3. Attendance List

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#### GORDON RESEARCH CONFERENCE

# "Fundamental Interactions of Water With Solid Surfaces" Kimball Union Academy, Meriden, New Hampshire

Theodore E. Madey, Chairman Rutgers University

Patricia A. Thiel. Vice Chairman Iowa State University

July 16-20, 1990

#### Sunday. July 15, 1990

7:00 p.m. Dinner 8:00 p.m. Mixer

### Monday, July 16, 1990

8:45 a.m. Introductory Remarks

Morning Session: Water-Metal Interactions

Carsten Benndorf, Discussion Leader

9:00 a.m. "Interaction of Water with Nickel and Peter Norton University of Western Ontario Aluminum Surfaces: Absolute

Coverages, Ordering and Dynamics"

9:50 a.m. Discussion

10:20 a.m. Coffee; Conference Photograph

10:40 a.m. Jose M. Heras "Water on Polycrystalline Metal

Surfaces" University Nacional de La Plata,

Argentina

11:30 a.m.

12:30 p.m.

Evening Session: Water Interactions With Additives

Galen B. Fisher, Discussion Leader

Lunch

Discussion

7:00 p.m. H. P. Bonzel "Alkali-Modified Adsorption of

KFA Julich Water"

Discussion 7:35 p.m.

J. M. White 8:00 p.m. "Surface Science of Coadsorbate

University of Texas Overlayers Involving Water"

Discussion 8:35 p.m.

# Tuesday. July 17. 1990

Morning Session: Theory of H<sub>2</sub>O Layers on Surfaces

Uzi Landman, Discussion Leader

9:00 a.m. Eckhard Spohr

University of California

"Computer Simulations of Water on

Metal Surfaces"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. J. Woods Halley, Jr.

University of Minnesota

"Electronic Structure and Dynamics at

the Water/Electrode Interface"

11:30 a.m. Discussion

12:30 p.m. Lunch

Evening Session: Water at Oxide Surfaces

Richard L. Kurtz, Discussion Leader

7:00 p.m. Victor E. Henrich

Yale University

"The Interaction of Water with Perfect

and Defect Surfaces of Semiconductors

and Oxides"

7:35 p.m. Discussion

7:50 p.m. Stephen H. Garofalini

Rutgers University

"Water Interactions with Oxide Glass

Surfaces - Molecular Dynamics

Simulations"

8:25 p.m. Discussion

8:40 p.m. Poster Session

# Wednesday, July 18, 1990

Morning Session: Electrochemical Aspects of Water-Surface Interactions

P. N. Ross, Jr., Discussion Leader

9:00 a.m. Eric Stuve

University of Washington

"In-Situ and Ex-Situ Studies of

Electrochemical Phenomena"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. Frederick T. Wagner "UHV Investigations of Surface

General Motors Research Labs

Solvation Effects in Electrochemistry"

11:30 a.m. Discussion

12:30 a.m. Lunch

### Evening Session: Interaction of Water With Electronic Materials

Patricia M. George, Discussion Leader

7:00 p.m. Yves Chabal

AT&T Bell Laboratories

"Infrared Spectroscopy of Water -

Modified Silicon Surfaces"

7:35 p.m. Discussion

7:50 p.m. J. D. Sinclair

AT&T Bell Laboratories

"The Role of Water in the Degradation

of Electronics: Materials, Mechanisms,

Protection, and Challenges"

8:25 p.m. Discussion

8:40 p.m. Poster Session

# Thursday, July 19, 1990

Morning Session: Interfacial Phenomena

Bruce Bunker, Discussion Leader

9:00 a.m. Brian Lawn

National Institute of Standards

and Technology

"Surface Forces, Adhesion and Fracture

of Brittle Solids"

9:50 a.m. Discussion

10:25 a.m. Coffee

10:40 a.m. John D. Porter

Univ. of California, Berkeley

"Interfacial Structure and Dynamics in

Hg/H2O/Hg Tunnel Junction Devices"

11:30 a.m. Discussion

12:30 p.m. Lunch

#### Evening Session: Wetting Phenomena

Mark O. Robbins, Discussion Leader

7:00 p.m. Michael Schick

University of Washington

"A Theoretical Overview of Wetting

Phenomena"

7:35 p.m. Discussion

8:00 p.m. Lawrence H. Dubois

AT&T Bell Laboratories

"Wetting of Organic Surfaces: Microscopic Predictions of a

Macroscopic Observable"

Discussion 8:35 p.m.

## Friday, July 20, 1990

Morning Session: Reactions of H<sub>2</sub>O at Surfaces

John T. Yates, Jr., Discussion Leader

8:45 a.m. Charles T. Campbell

University of Washington

"The Water-Gas Shift Reaction Over Clean and Cs-Promoted Cu Single-

Crystal Catalysts: Elementary

Processes"

9:35 a.m. Discussion

10:00 a.m. Coffee

10:15 a.m. Bengt Kasemo

Chalmers Univ. of Technology

"Water Formation and Decomposition

on Pt"

11:05 a.m. Discussion

12:00 noon Lunch

#### Posters Presented at Gordon Conference

#### "Fundamental Interactions of Water with Solid Surfaces"

#### Tuesday, July 17, 1990

Dr. G. Pirug
Institut für Grenzflächenforschung
Forschungszentrum Jülich GMBH
Postfach 1913
D-51170 Jülich 1
Federal Republic of Germany

"The Influence of Alkali Metals on the Oxidation of Si(100) Surfaces by H<sub>2</sub>0" (Authors: G. Pirug and H. P. Bonzel)

Dr. A. Brodsky
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

"Phase Transitions in Surface Water Layers"

Professor Jiri Skvarla

Department of Mineral Processing and Environmental Protection
Technical University
Park Komenskeho 19
043 84 Kosice
Czechoslovakia

"A Correlation Between the Wettability and Aggregation of Fine Minerals"

Robert Brosseau

Department of Chemistry
University of Montreal
Montreal, Quebec, CANADA

"Water on Pd(110)"
(Authors: R. Brosseau and T. H. Ellis)

Brian W. Callen
Department of Chemistry
University of Western Ontario
CANADA N6A 5B7

"Identification of Surface Water Molecules on Isotopically Substituted Ice Layers" (Authors: Brian W. Callen, K. Griffiths and P. R. Norton)

Professor J. A. Panitz
Department of Physics and
Astronomy
The University of New Mexico
Albuquerque, NM 87131

"Imaging Atom-Probe Studies of Aqueous Interfaces"

Eric K. Parks
Argonne National Laboratory
701 Lakeside Drive
Hinsdale, IL 60521

"Reactions of Water with Iron, Cobalt, and Nickel Clusters" (Authors: E. K. Parks, S. Riley, T. Klots and B. Winter) Stephen James Bushby
Department of Chemistry
University of Western Ontario
London, Ontario
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Si-Chung Chang
Department of Chemistry
Purdue University
West Lafayette, IN 47907-3699

Yitzhak Shnidman Research Laboratories Eastman Kodak Company Rochester, NY 14650-2109

W.-H. Hung
Department of Chemistry
Princeton University
Princeton, NJ 08544

#### Wednesday, July 18, 1990

Dr. Geoff Thornton Chemistry Department Manchester University Manchester M13 9PL United Kingdom

Dr. Rudolf Schubert Room 3X 215 Bellcore P. O. Box 7040 Red Bank, NJ 07701-7040

Dr. Richard Kurtz
Surface Science Division
National Institute for Science
and Technology
Gaithersburg, MD 20899

"Absolute Hydroxyl Coverage of Oxides Formed by Water Interaction with Al(100)" (Authors: S. J. Bushby, K. Griffiths, Z. H. Lu, D. K. Greber, R. S. Timsit and P. R. Norton)

"In-Situ Infrared Spectroscopy of Well-Defined Single Crystal Electrodes" (Authors: S.-C. Chang and M. Weaver)

"Concentration-Driven Surface Transition in the Wetting of Mixed Alkanethiol Monolayers" (Authors: Y. Shnidman, J. E. Eilers, S. D. Evans, R. Sharma, J. C. Chang and A. Ulman)

"The Adsorption of H<sub>2</sub>O on Clean and Oxidized Fe(100)"
(Authors: W.-H. Hung, J. Schwartz and S. L. Bernasek)

"H<sub>2</sub>O Adsorption on BSSCO (001) and Other Oxide Surfaces"

"The Effect of Relative Humidity on Electrical Contacts"

"The Role of Surface Defects in Water Chemisorption on TiO, (110)"

Dr. Ben Ocko
Department of Physics
Brookhaven National Laboratory
Upton, Long Island, NY 11973

"In-Situ X-ray Scattering Investigations of Electrode Surface Reconstructions"

Dr. Brian Maschhoff
Department of Physics
Laboratory for Surface Modification
Rutgers, The State University of
New Jersey
P. O. Box 849
Piscataway, NJ 08855-90849

"Interaction of Water with Insulator Surfaces" (Authors: Brian Maschhoff, J. M. Pan, M. Szymonski and T. E. Madey)

Dr. D. R. Baer Surface Physics Group Battelle Pacific NW Lab Battelle Blvd. Richland, WA 99352 "Interactions of H<sub>2</sub>O and Mn with the Cleavage Surface of CaCO<sub>3</sub>" (Authors: D. R. Baer, D. L. Blanchard and J. M. Zachara)

Prof. Andrej Wieckowski Department of Chemistry University of Illinois Urbana, IL 61801 "Voltammetry and Surface Science of Rh(100) and Rh(111) Surfaces"

Dr. Masakatsu Watanabe
Department of Chemistry
University of Pennsylvania
Philadelphia, PA 19104-6323

"Phase Transition of Water Between Metal Surfaces"

Dr. Fred Wagner
Physical Chemical Dept.
General Motors Research Labs
30500 Mound Road
Warren, MI 48090-9055

"Hydrogen and Water Coadsorption on Cu(110) and Pt(111): the Formation of  $H_3O$ ?"

Prof. J. Michael White Department of Chemistry University of Texas Austin, Texas 78712 "Optical Absorption of  $H_2O(g)$  and Amorphous Ice"

Dr. Patricia M. George Aerojet Electro Systems Surface and Contam. Dept. P. O. Box 296 Azusa, CA 91702 "The Reaction of Water on GaAs(100)"

Dr. Patricia M. George Aerojet Electro Systems Surface and Contam. Dept. P. O. Box 296 Azusa, CA 91702

Prof. Doug Doren
Department of Chemistry
University of Delaware
Newark, DE 19716

"An XPS Study of Water Removal from Be at 160K: Evidence for Ion Beam-Induced Oxidation"

"Molelcular Diffusion on Solid Surfaces: How Chemisorbed Molecules Differ from Atoms"

#### GORDON RESEARCH CONFERENCES

# FUNDAMENTAL INTERACTION OF WATER WITH SOLID SURFACES

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